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chain nodes :

 $7 \quad 8 \quad 9 \quad 10 \quad 11 \quad 12 \quad 13 \quad 14 \quad 15 \quad 16 \quad 17 \quad 24 \quad 25 \quad 26 \quad 27 \quad 28 \quad 29 \quad 30 \quad 31 \quad 32 \quad 33 \quad 40$ 41 48 49 52 53 54 55 56 57 58 59 60 61 62 63 65 64 ring nodes :  $1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 18 \quad 19 \quad 20 \quad 21 \quad 22 \quad 23 \quad 34 \quad 35 \quad 36 \quad 37 \quad 38 \quad 39 \quad 42$ 43 44 46 47 chain bonds : 1-13 2-14 3-7 4-11 5-12 6-9 7-8 7-17 9-10 9-15 9-1618-30 19-31 21-28 22-29 23-26 24-25 24-46 26-27 26-32 26-33 34-41 35-54 35-55 36 - 5236-53 37-58 37-59 38-40 39-56 39-57 42-62 42-63 43-49 44-64 44-65 45-48 47-60 47-61 ring bonds :  $1 - 2 \quad 1 - 6 \quad 2 - 3 \quad 3 - 4 \quad 4 - 5 \quad 5 - 6 \quad 18 - 19 \quad 18 - 23 \quad 19 - 20 \quad 20 - 21 \quad 21 - 22 \quad 22 - 23 \quad 34 - 35$ 34-39 35-36 36-37 37-38 38-39 42-43 42-47 43-44 44-45 45-46 46-47exact/norm bonds :  10/573,723 08/25/2009 STN: SEARCH

exact bonds :  $1-13 \quad 2-14 \quad 3-7 \quad 4-11 \quad 5-12 \quad 7-17 \quad 9-10 \quad 18-30 \quad 19-31 \quad 20-24 \quad 21-28 \quad 22-29 \quad 24-46$ 26-27 35-54 35-55 36-52 36-53 37-58 37-59 39-56 39-57 42-62 42-63 44-64 44-65 47-60 47-61 normalized bonds :  $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 18-19 \quad 18-23 \quad 19-20 \quad 20-21 \quad 21-22 \quad 22-23$ Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:Atom 35:CLASS 36:Atom 37:Atom 38:Atom 39:Atom 40:CLASS 41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 49:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:CLASS 64:CLASS 65:CLASS fragments assigned product role: containing 18 fragments assigned reactant/reagent role: containing 1 containing 34 L1STRUCTURE UPLOADED => FS L1 FULL FS IS NOT A RECOGNIZED COMMAND The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>). => S L1 FULL FULL SEARCH INITIATED 10:43:37 FILE 'CASREACT' SCREENING COMPLETE -2 REACTIONS TO VERIFY FROM 2 DOCUMENTS 100.0% DONE 2 VERIFIED 0 HIT RXNS 0 DOCS SEARCH TIME: 00.00.01 0 SEA SSS FUL L1 ( 0 REACTIONS) L2 => ---Logging off of STN---=> Executing the logoff script... => LOG Y

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124.09 124.31 FULL ESTIMATED COST

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